

# Construction of Darboux coordinates in noncanonical Hamiltonian systems via normal form expansions

Andrej Junginger, Jörg Main, and Günter Wunner

1. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

**Abstract.** Darboux's theorem guarantees the existence of local canonical coordinates on symplectic manifolds under certain conditions. We demonstrate a general method to construct such Darboux coordinates in the vicinity of a fixed point of a noncanonical Hamiltonian system via normal form expansions. The procedure serves as a tool to naturally extract canonical coordinates and at the same time to transform the Hamiltonian into its Poincaré-Birkhoff normal form. The method is general in the sense that it is applicable for arbitrary degrees of freedom, in arbitrary orders of the local expansion, and it is independent of the precise form of the Hamiltonian. The method presented allows for the general and systematic investigation of noncanonical Hamiltonian systems in the vicinity of fixed points, which e.g. correspond to ground, excited or transition states. As an exemplary field of application, we discuss a variational approach to quantum systems which defines a noncanonical Hamiltonian system for the variational parameters and which directly allows to apply transition state theory to quantum mechanical wave packets.

## 1. Introduction

It is at the core of physical sciences to describe and investigate the dynamics of physical systems. Depending on their nature, these can either be described by the Schrödinger equation in case of quantum mechanical systems, or e.g. in terms of Hamiltonian mechanics in case of a classical system. In both cases, a canonical structure of the dynamical equations is inherent which is expressed in the existence of conjugate pairs of field operators  $\hat{\psi}, \hat{\psi}^\dagger$  with infinite degrees of freedom or conjugate coordinates  $\mathbf{q}, \mathbf{p}$  with a finite number of degrees of freedom. Both approaches serve as powerful frameworks to investigate a huge amount of different physical problems. In addition to the global dynamics of a physical system which can be determined by solving the corresponding equations of motion, its fixed points play a crucial role in many investigations: For example, fixed points which correspond to a (local) minimum of the Hamiltonian form (metastable) ground states of the system. Moreover, fixed points which are related to saddle points of the Hamiltonian are unstable, excited states. A special class of such unstable fixed points are rank-1 saddle points which possess exactly one unstable direction. These points are of special interest in dynamical systems, because they form bottlenecks in the underlying phase space which separate different regions therein. Considering a dynamical system, the transition from one to the other subregion of phase space is then mediated by the saddle point. Therefore, the latter determines

the reaction dynamics between the different subregions which is the basic statement of transition state theory (see Refs. [1–7] and references therein).

Beyond the fixed points of the system’s dynamical equations themselves, their local properties are of high interest in many applications. For example, the local properties of a minimum of the Hamiltonian determine the physics of the system for small excitations from the ground state. Moreover, the local properties in the vicinity of a rank-1 saddle point or transition state determine the reaction dynamics and rates of the system. For a detailed analysis of the local fixed point properties of a canonical Hamiltonian system as well as for the construction of a dividing surface that separates reactants and products in it, a standard and powerful tool is its normal form expansion [7, 8]. If the Hamiltonian  $H$  is given in terms of a set of canonical coordinates  $\mathbf{q}, \mathbf{p}$  then the normal form of this Hamiltonian is given by

$$\tilde{H}(\mathbf{q}, \mathbf{p}) = \sum_{j=0}^{\infty} \frac{1}{j!} \text{ad}_W^j H(\mathbf{q}, \mathbf{p}), \quad (1)$$

where  $W$  is an appropriate generating function and  $\text{ad}_W H = \{W, H\}$  is the adjoint operator that equals the definition of the Poisson bracket (see Ref. [7] for details). By construction, the normal form (1) provides the most simple form of the original Hamilton function, while keeping all the essential properties of the dynamics.

In this paper, we focus on the local fixed point properties of the more general case of *noncanonical* Hamiltonian systems. In these the dynamical equations are Hamiltonian (see below for a precise definition), however, the underlying coordinates are not canonical. In such systems, fixed points and their local properties have the same physical meaning and importance as in the canonical case and for a detailed analysis of the local properties, it is desirable to obtain an analogue of the classical normal form also for the noncanonical system. However, the usual treatment (1) cannot be applied, because neither a classical Hamilton function in canonical coordinates nor such coordinates themselves are known. In this paper, we present a method by which both the transformation of a noncanonical Hamiltonian system into its normal form and simultaneously the construction of canonical coordinates is obtained. The result of the transformations is, by construction, a set of canonical normal form coordinates. In the latter, the energy functional of the system will serve as a classical Hamilton function which has the advantageous property that it is directly formulated in action variables.

Our paper is organized as follows: In Sec. 2, we introduce the general form of a noncanonical Hamiltonian system which is taken into account in this paper. Moreover, we discuss as a fixed point property of the linearised dynamical equations the latters’ general eigenvalue structure that will directly determine the normal form structure. In Sec. 3, the method to construct local canonical coordinates in the vicinity of the fixed point is introduced. Therefore, a symplectic basis formed by appropriately normalized eigenvectors of the linearised dynamical equations is used and higher-order terms of the expansions are treated via normal form transformations. As a key feature – and in contrast to the usual normal form expansion (1) of canonical Hamiltonians – this procedure treats the dynamical equations and the energy functional separately. Moreover, the normal form expansions are carried out in two steps: First, its polynomial structure is generated using the nonresonant terms of the corresponding generating function (see below for the latters’ definition). Second, the remaining resonant coefficients of the generating function which are free parameters are

chosen in such a way that the dynamical equations as well as the energy functional in normal form coordinates fulfil canonical equations, i.e. the normal form coordinates are canonical ones by construction. Finally, we discuss in Sec. 4 a variational approach to quantum systems which defines a noncanonical Hamiltonian system for the variational parameters.

## 2. Noncanonical Hamiltonian systems

Let us consider a Hamiltonian system with  $d$  degrees of freedom. In standard canonical coordinates  $\mathbf{u} = (q_1, p_1, \dots, q_d, p_d)^\top$ , the physics of this system is described by the Hamiltonian  $H = H(\mathbf{u})$  which is a real function of the coordinates. The dynamics of the system is then determined by Hamilton's equations

$$\mathcal{J}\dot{\mathbf{u}} = -\frac{\partial H(\mathbf{u})}{\partial \mathbf{u}}, \quad (2)$$

where,  $\mathcal{J}$  is the standard symplectic matrix

$$\mathcal{J} \equiv \begin{pmatrix} \mathcal{J}_1 & & 0 \\ & \ddots & \\ 0 & & \mathcal{J}_1 \end{pmatrix}, \quad \text{with} \quad \mathcal{J}_1 \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (3)$$

The latter relates the Hamiltonian vector field  $\dot{\mathbf{u}}$  to the derivative  $\partial H / \partial \mathbf{u}$  of the Hamiltonian, and it induces a symplectic geometry on phase space. As we have already mentioned in the introduction, such a canonical structure is also present in quantum mechanical Schrödinger systems, where the field operators  $\hat{\psi}, \hat{\psi}^\dagger$  play an analogous role to the conjugate coordinates  $\mathbf{q}, \mathbf{p}$ . However, this canonical structure is e.g. lost in case of a variational approach to quantum systems (see Sec. 4).

Therefore, we focus on the more general case of *noncanonical* Hamiltonian systems in this paper. Independent of the coordinates which are made use of, the latter can be defined in terms of differential geometry by the fact that the corresponding Hamiltonian vector field  $X_H$  is connected via an alternating, nondegenerate, and closed 2-form  $\omega^2(\cdot, \cdot)$  to the differential of a smooth function  $H$  on phase space [9], i.e.

$$\omega^2(X_H, \cdot) = dH. \quad (4)$$

Comparing this general definition with the standard canonical case discussed in Eq. (2), the matrix  $\mathcal{J}$  in Eq. (3) appears as a representation of the standard canonical 2-form  $\omega^2 = \sum_{i=1}^d dq_i \wedge dp_i$  in Eq. (4).

For the general case, a representation of Hamilton's equations (4) in noncanonical coordinates  $\mathbf{x} \in \mathbb{R}^{2d}$  can be written in the form

$$K(\mathbf{x}) \dot{\mathbf{x}} = -\frac{\partial E(\mathbf{x})}{\partial \mathbf{x}} \equiv -\mathbf{h}(\mathbf{x}). \quad (5)$$

Here,  $K$  is a skew-symmetric matrix ( $K_{ij} = -K_{ji}$ ),  $E$  is the energy functional of the system, and  $\mathbf{h}$  is defined as the latter's gradient. Note, that Eq. (5) is formally equivalent to Eq. (2), in the sense that the time derivative of the coordinates is related via a skew-symmetric matrix to the derivative of a real function which represents the energy of the system. What makes the system (5) noncanonical is the fact that the matrix  $K$  is not equal to the standard symplectic matrix  $\mathcal{J}$  defined in Eq. (3), but

it may have a more complicated structure. Especially,  $K$  is allowed to depend on the coordinates, i.e. the symplectic geometry may vary with position on the space of noncanonical coordinates  $\mathbf{x}$ . With these properties, the time-derivatives  $\dot{x}_i, \dot{x}_j$  of all coordinates ( $i, j = 1, \dots, 2d; i \neq j$ ) are, in general, coupled in a nontrivial way, and – in contrast to the canonical case – there do not exist preferential *pairs* of conjugate coordinates.

In order to investigate the geometric properties of the noncanonical coordinate space, we note that the matrix  $K$  naturally defines a differential 2-form

$$\omega^2 = \sum_{\substack{m,n=1 \\ m < n}}^{2d} K_{mn}(\mathbf{x}) dx_m \wedge dx_n. \quad (6)$$

This 2-form is alternating by definition of the wedge product which takes into account the skew-symmetry of  $K$ . Furthermore, the 2-form (6) is nondegenerate (i.e. for every  $dx_m \neq 0$  there exists a  $dx_n$  such that  $\omega^2 \neq 0$ ) if  $K$  is invertible. This is a natural assumption, because otherwise, the dynamical equations (5) cannot be solved for  $\dot{\mathbf{x}}$  uniquely. In addition, we assume that  $\omega^2$  is closed, i.e. its exterior derivative vanishes,

$$d\omega^2 = \sum_{\substack{m,n,k=1 \\ m < n}}^{2d} \frac{\partial K_{mn}(\mathbf{x})}{\partial x_k} dx_k \wedge dx_m \wedge dx_n = 0. \quad (7)$$

Whether or not the latter property is fulfilled will, in general, depend on the precise form of the matrix  $K$ . If these assumptions on the matrix  $K$  are fulfilled, then Darboux's theorem [10] guarantees the existence of local canonical coordinates. In the formulation of Arnold [11] the theorem reads:

Let  $\omega^2$  be a closed nondegenerate differential 2-form in a neighbourhood of a point in the space  $\mathbb{R}^{2d}$ . Then in some neighbourhood of this point one can choose a coordinate system  $(\mathbf{q}, \mathbf{p})$  such that the form has the standard form  $\omega^2 = \sum_{i=1}^d dq_i \wedge dp_i$ .

### 2.1. Local dynamical equations

The noncanonical Hamiltonian system (5) is the basis of all further considerations in this paper. As already mentioned in the introduction, we focus on its local dynamics in the vicinity of a fixed point. Thus, in the following, we will consider local Taylor expansions of  $K$  and  $\mathbf{h}$  at the fixed point up to any desired order  $n_{\max}$ ,

$$\left( \sum_{n=0}^{n_{\max}-1} K_n(\mathbf{x}) \right) \dot{\mathbf{x}} = - \sum_{n=1}^{n_{\max}} \mathbf{h}_n(\mathbf{x}), \quad (8)$$

where the matrix  $K$  and the vector  $\mathbf{h}$  are expanded independently according to

$$K(\mathbf{x}) \approx \sum_{n=0}^{n_{\max}-1} K_n(\mathbf{x}), \quad (9a)$$

$$\mathbf{h}(\mathbf{x}) \approx \sum_{n=1}^{n_{\max}} \mathbf{h}_n(\mathbf{x}). \quad (9b)$$

The terms  $K_n$  and  $\mathbf{h}_n$  summarize all terms of the respective expansion which are homogeneous of degree  $n$ , and  $\mathbf{h}_0 = 0$  vanishes because the expansion is performed at a fixed point. Alternatively, the expansion of the equations of motion (8) can be rewritten equivalently in the form

$$\dot{\mathbf{x}} = -K^{-1}(\mathbf{x}) \mathbf{h}(\mathbf{x}) \approx \sum_{n=1}^{n_{\max}} \mathbf{f}_n(\mathbf{x}), \quad (10)$$

where both  $K$  and  $\mathbf{h}$  are combined on the same side of the equation and where  $\mathbf{f}_n$  collects the terms of order  $n$ .

## 2.2. Local eigenvalue structure

For the following considerations, the local eigenvalue structure of the dynamical equations at a fixed point  $\dot{\mathbf{x}} = 0$  are of fundamental importance. These are determined by the linearised dynamical equations

$$K_0 \dot{\mathbf{x}} = -\mathbf{h}_1(\mathbf{x}) = F \mathbf{x}, \quad (11)$$

where it is assumed that the fixed point is located at the origin  $\mathbf{x} = 0$  for simplicity (this can always be achieved by a simple shift of the coordinates).  $K_0$  is the zeroth-order expansion of the matrix  $K$  and  $\mathbf{h}_1 = -F\mathbf{x}$  is the linearised vector  $\mathbf{h}$  at the fixed point. Because  $K$  is skew-symmetric in general, this property of course also holds for its zeroth-order approximation. The matrix  $F$  is symmetric, because it is the negative Hessian matrix of the energy functional according to Eq. (5),  $F_{mn} = -\partial^2 E / \partial x_m \partial x_n$ . Consequently, the equations

$$K_0 = -K_0^\top, \quad F = F^\top \quad (12)$$

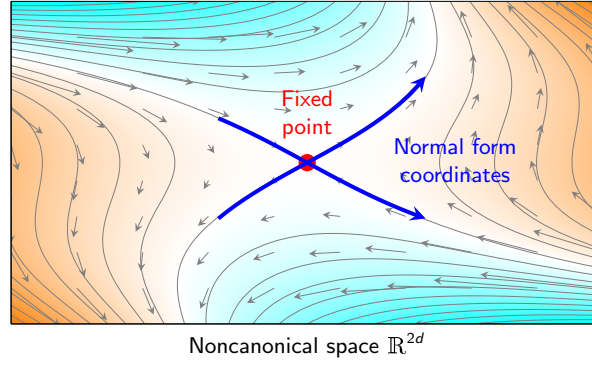
hold. In order to obtain the eigenvalue spectrum of the linearised equations of motion, the first-order differential equation (11) is solved using the ansatz  $\mathbf{x}(t) = \mathbf{v} e^{\lambda t}$ , where  $\lambda \in \mathbb{C}$  is a complex parameter, and  $\mathbf{v} \in \mathbb{C}^{2d}$  is a complex vector. Inserting this ansatz into Eq. (11), one obtains the generalized eigenvalue equation

$$F \mathbf{v} = \lambda K_0 \mathbf{v}. \quad (13)$$

The eigenvalues  $\lambda$  are the roots of the characteristic polynomial  $\chi(\lambda) = \det(F - \lambda K_0)$ , and with the properties (12), it can easily be shown that the characteristic polynomial is an even function of  $\lambda$ , i.e.  $\chi(\lambda) = \chi(-\lambda)$ . Thus, if  $\lambda$  is a root of the characteristic polynomial, then also  $-\lambda$  is a root, so that all the eigenvalues occur pairwise with different sign. Therefore, the eigenvalue spectrum of the linearised dynamical equations in the vicinity of a fixed point always exhibits the structure

$$\boldsymbol{\lambda}^\pm = (+\lambda_1, -\lambda_1, \dots, +\lambda_d, -\lambda_d) \quad (14)$$

which will be of fundamental importance for the normal form expansions performed in the next Sec. 3.



**Figure 1.** Schematic illustration of the normal form coordinates. The contour lines represent isosurfaces of the energy functional  $E$  and the arrows depict the vector field  $\dot{\mathbf{x}}$  obtained by the dynamical equations (5). In the vicinity of a fixed point (red circle), the normal form coordinates define a local coordinate system whose origin is the fixed point.

### 3. Construction of canonical normal form coordinates

The knowledge of canonical coordinates is fundamental to many methods known from classical Hamiltonian mechanics and, beyond their existence, a central question is how these can be constructed. As the key result of this paper, a general method to construct canonical normal form coordinates will be presented in this section. As will be shown, this method has the advantage that it simultaneously yields both a procedure to extract canonical coordinates and a transformation of the system into its Poincaré-Birkhoff normal form. The procedure consists of the following three steps (see Fig. 1):

- (i) In the first step, the expansions (9) as well as that of the energy functional  $E$  are transformed via a linear change of coordinates to a symplectic basis which is defined by the eigenvectors of the linearised dynamical equations. The resulting diagonal coordinates are canonical ones in the first order of the expansions.
- (ii) Successive Lie transforms are applied order by order to treat the higher-order corrections of the expansions. In the corresponding generating function two different types of terms will be distinguished, namely “nonresonant” and “resonant” coefficients (see below). The generation of the normal form structure will be performed via the nonresonant terms, and all of them are determined uniquely by the requirement that certain monomials of the dynamical equations shall be removed. Which of the terms remain after the Lie transforms is solely determined by a resonance condition depending on the eigenvalues, and because of their general structure (14), the normal form will exhibit a fundamental polynomial structure.
- (iii) The normal form expansions leave the freedom to choose the resonant terms of the generating function. In the last step, these free parameters are chosen in a way that the dynamical equations and the energy functional fulfil canonical equations, i.e. the normal form coordinates are canonical ones by construction.

### 3.1. Symplectic basis

In order to “simplify” the system in its lowest order, it is sufficient to focus on the linearised dynamical equations (11). A natural basis of this linearised system is spanned by its eigenvectors  $\mathbf{v}_{2i-1}, \mathbf{v}_{2i}$ . These are solutions of the generalized eigenvalue problem

$$F \mathbf{v}_{2i-1} = +\lambda_i K_0 \mathbf{v}_{2i-1}, \quad (15a)$$

$$F \mathbf{v}_{2i} = -\lambda_i K_0 \mathbf{v}_{2i}, \quad (15b)$$

where  $i = 1, \dots, d$ . The normalization of the eigenvectors is basically free, however, it is appropriate to fix the normalization by requiring that

$$\langle \mathbf{v}_{2i-1} | K_0 | \mathbf{v}_{2i} \rangle = -\langle \mathbf{v}_{2i} | K_0 | \mathbf{v}_{2i-1} \rangle = 1, \quad (16a)$$

$$\langle \mathbf{v}_{2i-1} | F | \mathbf{v}_{2i} \rangle = \langle \mathbf{v}_{2i} | F | \mathbf{v}_{2i-1} \rangle = \lambda_i \quad (16b)$$

for all  $i = 1, \dots, d$ . Combining the eigenvectors in the transformation matrix  $T = (\mathbf{v}_1, \dots, \mathbf{v}_{2d})$ , the choice (16) by construction guarantees the block structures

$$T^\top K_0 T = \mathcal{J} \quad \text{and} \quad T^\top F T = \begin{pmatrix} 0 & \lambda_1 & & & \\ \lambda_1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & \lambda_d \\ & & & \lambda_d & 0 \end{pmatrix}, \quad (17)$$

where  $\mathcal{J}$  is the standard symplectic matrix defined in Eq. (3). Consequently, the normalized eigenvectors define a symplectic basis and the coordinates are canonical ones concerning the linearised system.

In order to regard the full, nonlinearised dynamical equations in this symplectic basis, the transformation  $\mathbf{x} \rightarrow \mathbf{x}' = T^{-1} \mathbf{x}$  needs to be applied also to the higher-order terms. Emanating from Eq. (10) and omitting the prime, this linear change of coordinates transforms the dynamical equations into the form

$$\dot{\mathbf{x}} = T^{-1} \sum_{n=1}^{n_{\max}} \mathbf{f}_n(T\mathbf{x}) \equiv \mathbf{a}(\mathbf{x}) = \sum_{n=1}^{n_{\max}} \mathbf{a}_n(\mathbf{x}). \quad (18)$$

In the last step, the single expansion coefficients have been redefined by the coefficients  $\mathbf{a}_n$  which collect the terms homogeneous of degree  $n$ . It is noted that, because the inverse matrix  $T^{-1}$  is used here instead of the transpose  $T^\top$ , the linear term of Eq. (18) is diagonal by construction,

$$\mathbf{a}_1(\mathbf{x}) = (T^{-1} F T) \mathbf{x} = \begin{pmatrix} +\lambda_1 & & & & \\ & -\lambda_1 & & & \\ & & \ddots & & \\ & & & +\lambda_d & \\ & & & & -\lambda_d \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{2d-1} \\ x_{2d} \end{pmatrix}. \quad (19)$$

Note that the originally real vector field (10) is, in general, transformed into a complex one ( $\mathbf{a}_n \in \mathbb{C}^{2d}$ ) by the diagonalisation, if the eigenvalue spectrum includes imaginary terms. Analogously to the dynamical equations, also the energy functional is expanded

in the vicinity of the fixed point, and the linear transformation  $\mathbf{x} \rightarrow \mathbf{x}' = T^{-1}\mathbf{x}$  is applied. This results in the scalar field

$$E(\mathbf{x}) = \sum_{n=0}^{n_{\max}+1} E_n(\mathbf{x}), \quad (20)$$

whose coefficients, again, become complex in general, and whose second-order term has the structure  $E_2 = \sum_{i=1}^d \lambda_i x_{2i-1} x_{2i}$ .

### 3.2. Normal form transformations – nonresonant terms

The diagonalisation of the local dynamical equations as described in the previous section 3.1, simplifies their linear part in a way that it becomes diagonal. However, for the terms of higher order, a “simplification” cannot be achieved by this step. For this purpose, a normal form expansion of the diagonalized dynamical equations (18) is performed in this section making use of successive Lie transforms. The general treatment of local dynamical systems and their normal forms has been described by Murdock [8] in detail. Here, it is applied to the  $2d$ -dimensional local dynamical equations (18) with their special eigenvalue structure (14).

In order to bring the local equations of motion into normal form, a nonlinear near-identity transformation

$$\mathbf{x} = \phi_\varepsilon(\mathbf{y}) \quad (21)$$

is applied, which transforms from the “old” coordinates  $\mathbf{x}$  to “new” ones  $\mathbf{y}$ , and which is differentiable in the new coordinates  $\mathbf{y}$  as well as in the parameter  $\varepsilon$ . The latter serves as a continuous scaling parameter that is introduced in a way that for  $\varepsilon = 0$  one obtains the identity transformation, while the finally desired transformation is obtained for  $\varepsilon = 1$ ,

$$\mathbf{x} = \phi_{\varepsilon=0}(\mathbf{y}) = \mathbf{y}, \quad (22a)$$

$$\mathbf{x} = \phi_{\varepsilon=1}(\mathbf{y}) = \phi(\mathbf{y}). \quad (22b)$$

Instead of providing the explicit function (21), the change of coordinates is defined implicitly, by the requirement that it is the solution of the differential equation

$$\frac{d\mathbf{x}}{d\varepsilon} = \mathbf{g}(\mathbf{x}), \quad (23)$$

with  $\mathbf{g}$  being the generating function of the transformation. As it is shown in Ref. [8], the final change of variables (22b) transforms a vector field  $\mathbf{a}$  defining the differential equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{a}(\mathbf{x}) \quad (24)$$

into a vector field  $\mathbf{b}$  in the new coordinates  $\mathbf{y}$  with

$$\frac{d\mathbf{y}}{dt} = \mathbf{b}(\mathbf{y}). \quad (25)$$

The connection between the two vector fields is

$$\mathbf{b}(\mathbf{y}) = \sum_{j=0}^{\infty} \frac{1}{j!} \mathcal{L}_{\mathbf{g}}^j \mathbf{a}(\mathbf{x})|_{\mathbf{x}=\mathbf{y}}, \quad (26)$$



where  $\mathcal{L}_g$  is the *homological operator* acting on differentiable vector fields according to

$$\mathcal{L}_g \mathbf{a}(\mathbf{x}) \equiv \frac{\partial \mathbf{a}(\mathbf{x})}{\partial \mathbf{x}} \mathbf{g}(\mathbf{x}) - \frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x}} \mathbf{a}(\mathbf{x}). \quad (27)$$

Analogously, the same generating function transforms the energy functional according to

$$\tilde{E}(\mathbf{y}) = \sum_{j=0}^{\infty} \frac{1}{j!} \mathcal{D}_g^j E(\mathbf{x})|_{\mathbf{x}=\mathbf{y}}. \quad (28)$$

Here, the *right-multiplication operator*  $\mathcal{D}_g$  is defined by

$$\mathcal{D}_g E(\mathbf{x}) \equiv \frac{\partial E(\mathbf{x})}{\partial \mathbf{x}} \mathbf{g}(\mathbf{x}). \quad (29)$$

*3.2.1. Transformation of multivariate polynomials* As already mentioned above, the local dynamical equations as well as the energy functional are on hand in the form of a formal power series or local Taylor expansion, i.e. as a multivariate polynomial. Therefore, it is convenient to also define the generating function as a multivariate polynomial, so that the transformed fields will also be such ones. In the following, these polynomials are written as

$$\mathbf{a}(\mathbf{x}) = \sum_{n=1}^{n_{\max}} \mathbf{a}_n(\mathbf{x}) = \sum_{|\mathbf{m}|=1}^{n_{\max}} \boldsymbol{\alpha}_{\mathbf{m}} \mathbf{x}^{\mathbf{m}}, \quad (30a)$$

$$\mathbf{b}(\mathbf{x}) = \sum_{n=1}^{n_{\max}} \mathbf{b}_n(\mathbf{x}) = \sum_{|\mathbf{m}|=1}^{n_{\max}} \boldsymbol{\beta}_{\mathbf{m}} \mathbf{x}^{\mathbf{m}}, \quad (30b)$$

$$\mathbf{g}(\mathbf{x}) = \sum_{n=1}^{n_{\max}} \mathbf{g}_n(\mathbf{x}) = \sum_{|\mathbf{m}|=1}^{n_{\max}} \boldsymbol{\gamma}_{\mathbf{m}} \mathbf{x}^{\mathbf{m}}, \quad (30c)$$

$$E(\mathbf{x}) = \sum_{n=0}^{n_{\max}+1} E_n(\mathbf{x}) = \sum_{|\mathbf{m}|=0}^{n_{\max}+1} \xi_{\mathbf{m}} \mathbf{x}^{\mathbf{m}}, \quad (30d)$$

where  $\mathbf{a}_n, \mathbf{b}_n, \mathbf{g}_n, E_n$  denote the terms of the respective series which are homogeneous of degree  $n$ , and  $\boldsymbol{\alpha}_{\mathbf{m}}, \boldsymbol{\beta}_{\mathbf{m}}, \boldsymbol{\gamma}_{\mathbf{m}}, \xi_{\mathbf{m}}$  are the coefficients of the expansion. Furthermore, the multi-index notation

$$\mathbf{x}^{\mathbf{m}} = x_1^{m_1} x_2^{m_2} \dots x_{2d}^{m_{2d}}, \quad (31a)$$

$$|\mathbf{m}| = m_1 + m_2 + \dots + m_{2d} \quad (31b)$$

with the integer vector  $\mathbf{m} \in \mathbb{N}_0^{2d}$  is used. The purpose of the following normal form transformation is that – for given expansion coefficients  $\boldsymbol{\alpha}_{\mathbf{m}k}$  and  $\xi_{\mathbf{m}k}$  – the coefficients  $\boldsymbol{\gamma}_{\mathbf{m}k}$  of the generating function are chosen in such a way that as many as possible of the resulting coefficients  $\boldsymbol{\beta}_{\mathbf{m}k}$  vanish, and that they are connected to the energy functional via canonical equations.

As the following discussion will show, it is possible to perform the transformations order by order, because one can specifically transform the  $n$ -th order of the original vector field  $\mathbf{a}_n$ , if the generating function is chosen to be homogeneous of degree  $n$ ,

$$\mathbf{g}(\mathbf{x}) = \mathbf{g}_n(\mathbf{x}) = \sum_{|\mathbf{m}|=n} \boldsymbol{\gamma}_{\mathbf{m}} \mathbf{x}^{\mathbf{m}}. \quad (32)$$

Inserting the multivariate polynomials (30) with the constraint (32) for the generating function into Eq. (26), one obtains, after renaming  $\mathbf{y}$  by  $\mathbf{x}$ , the homological equation

$$\mathbf{b}_n(\mathbf{x}) = \mathbf{a}_n(\mathbf{x}) + \mathcal{L}_{\mathbf{g}_n} \mathbf{a}_1(\mathbf{x}) \quad (33)$$

for the transformation of the monomials which are equal to the degree of the generating function. From this, the transformation of the single coefficients can be extracted. For the  $k$ -th component ( $k = 1, 2, \dots, 2d$ ) it reads

$$\beta_{\mathbf{m}k} = \alpha_{\mathbf{m}k} + (\lambda_k^\pm - \langle \mathbf{m}, \boldsymbol{\lambda}^\pm \rangle) \gamma_{\mathbf{m}k}. \quad (34)$$

where  $\langle \mathbf{m}, \boldsymbol{\lambda}^\pm \rangle$  is the standard scalar product.

A prior purpose of the above described transformations is to eliminate as many monomials as possible in the original multivariate polynomial. One can see from Eq. (34) that a nonvanishing monomial ( $\alpha_{\mathbf{m}k} \neq 0$ ) can be eliminated ( $\beta_{\mathbf{m}k} = 0$ ) by the Lie transform with an appropriate choice of the generating function, if the eigenvalue  $\lambda_k^\pm$  is “nonresonant”, i.e. if

$$\lambda_k^\pm - \langle \mathbf{m}, \boldsymbol{\lambda}^\pm \rangle \neq 0. \quad (35a)$$

Otherwise, if the condition of resonance

$$\lambda_k^\pm - \langle \mathbf{m}, \boldsymbol{\lambda}^\pm \rangle = 0 \quad (35b)$$

is fulfilled, the respective term cannot be eliminated. It is noted that, in the following, monomials  $\mathbf{x}^{\mathbf{m}}$  whose integer vector  $\mathbf{m}$  fulfils Eq. (35a) are referred to as “nonresonant monomials” and those fulfilling Eq. (35b) are called “resonant monomials”. Analogously, their coefficients are referred to as nonresonant and resonant coefficients, respectively. Finally, the polynomial is said to be in normal form with respect to its linear part  $\mathbf{a}_1$ , if only monomials fulfilling Eq. (35b) are left.

The final polynomial structure of the normal form of the local dynamical equations is determined by the eigenvalues of the linearised equations of motion, because only monomials fulfilling Eq. (35b) remain after the Lie transforms. Moreover, due to the fact that these eigenvalues exhibit the general structure (14) of pairwise eigenvalues with different sign, the normal form also possesses a general polynomial structure. Denoting the entries of the integer vector by  $\mathbf{m} = (m_1, m_2, \dots, m_{2d})^\top$ , the condition of resonance (35b) becomes ( $i = 1, 2, \dots, d$ )

$$[\lambda_1(m_1 - m_2) + \lambda_2(m_3 - m_4) + \dots + \lambda_d(m_{2d-1} - m_{2d})] = \pm \lambda_i, \quad (36)$$

where the upper sign is valid for  $k = 2i - 1$  and the lower one for  $k = 2i$ . Assuming rational independence,  $\lambda_i/\lambda_j \notin \mathbb{Q}$ , of all pairs of eigenvalues  $i \neq j$ , Eq. (36) is fulfilled if and only if

$$m_{2i-1} = m_{2i} \pm 1, \quad (i = 1, 2, \dots, d), \quad (37a)$$

$$m_{2j-1} = m_{2j}, \quad (j \neq i). \quad (37b)$$

Because of Eqs. (37), the monomials which remain in the vector field after the Lie transforms exhibit a general structure and each order  $n$  of the normal form can be

**Table 1.** Illustration of the fundamental polynomial structure of the dynamical equations (38) and the energy functional (41) for a system with  $d = 2$  degrees of freedom. In normal form coordinates, there remain only terms with odd degree of the monomial in the equations of motion. Moreover, the exponents of the variables  $x_{2i-1}, x_{2i}$  in the respective component of the vector field differ by one and the terms  $x_{2j-1}, x_{2j}$  with  $j \neq i$  (displayed in brackets) have the same exponent. By contrast, the energy functional only consists of monomials with even degree and all variables  $x_{2j-1}, x_{2j}$  occur in products. The extension of this structure to  $d > 2$  degrees of freedom is straightforward. In this case, additional terms  $(x_5 x_6), (x_7 x_8), \dots$  occur in the expansions.

Field	Degree $n$ of the monomial						
	0	1	2	3	4	5	6
$\dot{x}_1$	–	$x_1$	–	$x_1^2 x_2^1 (x_3 x_4)^0$ $x_1^1 x_2^0 (x_3 x_4)^1$	–	$x_1^3 x_2^2 (x_3 x_4)^0$ $x_1^2 x_2^1 (x_3 x_4)^1$ $x_1^1 x_2^0 (x_3 x_4)^2$	–
$\dot{x}_2$	–	$x_2$	–	$x_1^1 x_2^2 (x_3 x_4)^0$ $x_1^0 x_2^1 (x_3 x_4)^1$	–	$x_1^2 x_2^3 (x_3 x_4)^0$ $x_1^1 x_2^2 (x_3 x_4)^1$ $x_1^0 x_2^1 (x_3 x_4)^2$	–
$\dot{x}_3$	–	$x_3$	–	$x_3^2 x_4^1 (x_1 x_2)^0$ $x_3^1 x_4^0 (x_1 x_2)^1$	–	$x_3^3 x_4^2 (x_1 x_2)^0$ $x_3^2 x_4^1 (x_1 x_2)^1$ $x_3^1 x_4^0 (x_1 x_2)^2$	–
$\dot{x}_4$	–	$x_4$	–	$x_3^1 x_4^2 (x_1 x_2)^0$ $x_3^0 x_4^1 (x_1 x_2)^1$	–	$x_3^2 x_4^3 (x_1 x_2)^0$ $x_3^1 x_4^2 (x_1 x_2)^1$ $x_3^0 x_4^1 (x_1 x_2)^2$	–
$E$	const.	–	$(x_1 x_2)^1$ $(x_3 x_4)^1$	–	$(x_1 x_2)^2 (x_3 x_4)^0$ $(x_1 x_2)^1 (x_3 x_4)^1$ $(x_1 x_2)^0 (x_3 x_4)^2$	–	$(x_1 x_2)^3 (x_3 x_4)^0$ $(x_1 x_2)^2 (x_3 x_4)^1$ $(x_1 x_2)^1 (x_3 x_4)^2$ $(x_1 x_2)^0 (x_3 x_4)^3$

written as

$$b_{n(2i-1)} = \sum_{\substack{\mathbf{m} \in \mathcal{M}, \\ |\mathbf{m}|=n+1, \\ \text{nonneg.}}} \beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)} \mathbf{x}^{[\mathbf{m}-\hat{\mathbf{e}}_{2i}]}, \quad (38a)$$

$$b_{n(2i)} = \sum_{\substack{\mathbf{m} \in \mathcal{M}, \\ |\mathbf{m}|=n+1, \\ \text{nonneg.}}} \beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2i-1}](2i)} \mathbf{x}^{[\mathbf{m}-\hat{\mathbf{e}}_{2i-1}]}. \quad (38b)$$

with  $i = 1, 2, \dots, d$ . Here, the summation is carried out over the set

$$\mathcal{M} \equiv \{ \mathbf{m} \in \mathbb{N}^{2d} \mid m_{2j-1} = m_{2j}; j = 1, 2, \dots, d \}, \quad (39)$$

which is defined by Eq. (37b) and the unit vectors  $\hat{\mathbf{e}}_{2i-1}$  and  $\hat{\mathbf{e}}_{2i}$  take into account the term  $\pm 1$  in Eq. (37a). Moreover, the constraint “nonneg.” in the summation denotes to add only those terms for which the indices  $[\mathbf{m} - \hat{\mathbf{e}}_{2i}]$  and  $[\mathbf{m} - \hat{\mathbf{e}}_{2i-1}]$  only have nonnegative entries, i.e. those  $\mathbf{m} \in \mathcal{M}$  with  $m_{2i-1} = m_{2i} = 0$  are not taken into account. An equivalent interpretation of this constraint is to set all terms  $\beta_{\mathbf{m}k}$  to zero, if its index  $\mathbf{m}$  possesses at least one negative entry.

Concluding, in normal form coordinates, the variables  $x_{2i-1}, x_{2i}$  in the respective component of the dynamical equations occur with exponents which differ exactly by

one, while the terms  $x_{2j-1}, x_{2j}$  with  $j \neq i$  have the same exponent (cf. Table 1). Note that all monomials remaining in Eqs. (38) are of odd degree. All terms of even degree have been eliminated completely by the Lie transforms, because the condition of resonance (35b) cannot be fulfilled, if  $|\mathbf{m}|$  is even.

### 3.2.2. Determination of the generating function to eliminate the nonresonant terms

After having discussed the general structure of the normal form, its actual calculation is presented in this section. The calculation will be carried out order by order, i.e. the orders  $n = 2, 3, 4, \dots$  are treated successively. It is assumed that the system is already in normal form up to the order  $n - 1$ . Then, a generating function  $\mathbf{g}_n$  is constructed to transform the  $n$ -th order of the equations of motion.

As already mentioned above, the coefficients  $\gamma_{\mathbf{m}k}$  of the generating function which are nonresonant, i.e. Eq. (35a) is valid, can be chosen in such a way that the corresponding term  $\alpha_{\mathbf{m}k}$  of the original expansion is eliminated. Such nonresonant coefficients occur in every order of the expansion. In particular, the generating function of each even degree  $n$  only consists of nonresonant coefficients. The determination of the nonresonant coefficients  $\gamma_{\mathbf{m}k}$  of the generating function is straightforward. Since their purpose is to eliminate the original term  $\alpha_{\mathbf{m}k}$ , they are uniquely determined by Eq. (34). Requiring  $\beta_{\mathbf{m}k} = 0$  and solving for the coefficient of the generating function (32), one obtains

$$\gamma_{\mathbf{m}k} = \begin{cases} \frac{\alpha_{\mathbf{m}k}}{\langle \mathbf{m}, \boldsymbol{\lambda}^\pm \rangle - \lambda_k^\pm}, & \text{if } \lambda_k^\pm - \langle \mathbf{m}, \boldsymbol{\lambda}^\pm \rangle \neq 0, \\ c_{\mathbf{m}k}, & \text{else.} \end{cases} \quad (40)$$

The choice in the first line guarantees the elimination of the term  $\alpha_{\mathbf{m}k}$  in the nonresonant case. All the resonant terms are free parameters, which do not change the  $\beta_{\mathbf{m}k}$  of the order  $|\mathbf{m}| = n$ . For simplicity these terms are set to  $c_{\mathbf{m}k} = 0$  in the transformations of the nonresonant coefficients and their final determination will be treated separately (see Sec. 3.3).

After the nonresonant terms of the generating function have been determined according to Eq. (40), the corresponding transformation is applied to the equations of motion and to the energy functional, i.e. Eqs. (26) and (28) are evaluated. As a result, the polynomial structure of the equations of motion takes the form (38) up to the order  $n$  of the transformation. Furthermore, the generating function  $\mathbf{g}_n$  transforms the order  $n + 1$  of the energy functional into the structure (cf. Table 1)

$$E_{n+1}(\mathbf{x}) = \sum_{\substack{\mathbf{m} \in \mathcal{M} \\ |\mathbf{m}| = n+1}} \xi_{\mathbf{m}} \mathbf{x}^{\mathbf{m}}. \quad (41)$$

Note that this polynomial structure of the energy functional, i.e. the fact that only terms  $\mathbf{m} \in \mathcal{M}$  occur in the expansion, does not directly follow from the definition of the generating function. This structure is a result of Darboux's theorem which guarantees the existence of canonical coordinates, because any polynomial structure differing from that in Eq. (41) would violate the theorem.

### 3.3. Normal form transformations – resonant terms

In normal form coordinates the dynamical equations (38) and the energy functional (41) naturally exhibit a polynomial structure that allows for the identification of the

normal form coordinates as canonical ones according to the canonical equation

$$\mathbf{b}_n(\mathbf{x}) = \mathcal{J} \frac{\partial}{\partial \mathbf{x}} E_{n+1}(\mathbf{x}) \quad (42)$$

with the energy functional acting as Hamiltonian. Equation (42) is valid in each order  $n$ , if the coefficients  $\beta_{\mathbf{m}k}$  and  $\xi_{\mathbf{m}}$  in Eqs. (38) and (41) fulfil the conditions

$$m_{2i}\xi_{\mathbf{m}} = \beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)}, \quad (43a)$$

$$\beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)} = -\beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2i-1}](2i)}, \quad (43b)$$

$$\frac{\beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)}}{m_{2i}} = \frac{\beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2j}](2j-1)}}{m_{2j}} \quad (43c)$$

for all  $i, j = 1, 2, \dots, d$  ( $i \neq j$ ) and  $\mathbf{m} \in \mathcal{M}$  with  $|\mathbf{m}| = n + 1$ . Here, Eq. (43a) is the requirement that the coefficients of the dynamical equations and those of the energy functional are connected via derivatives according to Eqs. (42). The sign structure of the symplectic matrix  $\mathcal{J}$  is taken into account by Eq. (43b) for each pair  $x_{2i-1}, x_{2i}$  of “conjugate coordinates”, and Eq. (43c) considers the fact that terms in the expansion of *different* pairs  $x_{2i-1}, x_{2i}$  and  $x_{2j-1}, x_{2j}$  ( $i \neq j$ ) result from the *same* term of the energy functional.

As a consequence of the normal form expansion together with the general eigenvalue structure (14), Eq. (43b) is fulfilled after the Lie transforms have been applied as discussed in Sec. 3.2. However, the conditions (43a) and (43c) are *not* fulfilled, in general. This is due to the fact that – although the polynomial structure of the expansions is uniquely determined by the eigenvalue structure – the explicit normal form, i.e. the coefficients of the expansion, are not unique. The reason is that the resonant coefficients  $c_{\mathbf{m}k}$  of the generating function in Eq. (40) are free, and that the choice to set them zero does not guarantee the fulfilment of all Eqs. (43). Therefore, further steps are necessary in order to guarantee that the latter are valid, and these steps are presented in the following.

We emphasize that it is precisely this treatment of the resonant terms of the generating function which is the difference between the usual normal form procedure of canonical Hamiltonians and the transformation of the noncanonical system: If the coordinates had been canonical at the beginning, the choice  $c_{\mathbf{m}k} = 0$  in Eq. (40) would have kept this property. Vice versa, we will use an appropriate choice  $c_{\mathbf{m}k} \neq 0$  in the following to generate canonical coordinates.

*3.3.1. Particular choice of the resonant generating function and the corresponding transformations* Resonant terms occur in every odd order  $n = 3, 5, 7, \dots$  of the generating function (32), and a fundamental property of them is the fact that they do not affect the polynomial structure of the expansions, but they only modify their coefficients. Vice versa, this property can be used in order to guarantee the fulfilment of the canonical equations (43) by a suitable choice of the resonant terms as it will be demonstrated in the following. For this purpose, it is investigated in detail in this section how a resonant generating function of degree  $n$  transforms the next-higher order terms of the dynamical equations as well as the energy functional. Finally, Eqs. (43) will serve as conditional equations for the determination of the resonant coefficients.

In a resonant generating function of degree  $n$ , there occur coefficients  $\gamma_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)}$  and  $\gamma_{[\mathbf{m}-\hat{\mathbf{e}}_{2i-1}](2i)}$  with  $\mathbf{m} \in \mathcal{M}$  and  $|\mathbf{m}| = n + 1$ , i.e. there is exactly one

term corresponding to each of the monomials remaining in the dynamical equations (38). In order to guarantee that Eqs. (43) hold for the whole expansion, it will be sufficient only to consider the terms  $\gamma_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)}$  and to set  $\gamma_{[\mathbf{m}-\hat{\mathbf{e}}_{2i-1}](2i)} = 0$  for simplicity. With this choice, the resonant generating function homogeneous of degree  $n$  has the form

$$g_{n(2i-1)}(\mathbf{x}) = \sum_{\substack{\mathbf{m} \in \mathcal{M}, \\ |\mathbf{m}|=n+1, \\ \text{nonneg.}}} \gamma_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)} \mathbf{x}^{[\mathbf{m}-\hat{\mathbf{e}}_{2i}]}, \quad (44a)$$

$$g_{n(2i)}(\mathbf{x}) = 0. \quad (44b)$$

It is easily verified from Eq. (29) that the  $j$ -fold application  $\mathcal{D}_{\mathbf{g}_n}^j E_k$  of the right-multiplication operator with a generating function homogeneous of degree  $n$  onto the part of the energy functional of degree  $k$  results in a polynomial homogeneous of degree  $k + j(n-1)$ . Furthermore, the lowest order which is affected in Eq. (28) is  $n+1$ . Consequently, there are two cases which contribute to the order  $n+1$  of the transformed field, namely those with  $k + j(n-1) \stackrel{!}{=} n+1$ . On the one hand, this is the contribution  $k = n+1$  and  $j = 0$ , on the other hand it is  $k = 2$  and  $j = 1$ , so that the precise transformation reads

$$\tilde{E}_{n+1}(\mathbf{x}) = E_{n+1}(\mathbf{x}) + \mathcal{D}_{\mathbf{g}_n} E_2(\mathbf{x}), \quad (45)$$

where  $\tilde{E}_{n+1} = \sum_{|\mathbf{m}|=n+1} \tilde{\xi}_{\mathbf{m}} \mathbf{x}^{\mathbf{m}}$  is the transformed field. Inserting the expansions (30) into Eq. (45), and using the fact that the second order of the energy functional has the form  $E_2 = \sum_{i=1}^d \lambda_i x_{2i-1} x_{2i}$  in normal form coordinates, Eq. (45) can directly be reformulated in terms of the energy functional's coefficients:

$$\tilde{\xi}_{\mathbf{m}} = \xi_{\mathbf{m}} + \sum_{\substack{i=1, \\ \text{nonneg.}}}^d \lambda_i \gamma_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)}. \quad (46)$$

Analogously, the effect of a resonant generating function onto the dynamical equations can be investigated. If the latter are already in their normal form (38), there are only odd degrees of the expansion  $\mathbf{b}_1, \mathbf{b}_3, \mathbf{b}_5, \dots$  left as discussed above. By definition, the first-order term  $\mathbf{b}_1$  containing the eigenvalues does not contribute to the Lie operator for a resonant generating function, i.e.  $\mathcal{L}_{\mathbf{g}_n} \mathbf{b}_1 = 0$ . This identity directly follows from Eq. (34), because the resonant coefficients are always multiplied by zero. Therefore, the lowest-order term which leads to a contribution of the Lie operator is the term  $\mathbf{b}_3$ . From Eq. (26) it follows that the lowest-order term which is modified by a resonant generating function of degree  $n$  together with  $\mathbf{b}_3$  is the order  $n+2$  of the dynamical equations,

$$\tilde{\mathbf{b}}_{n+2}(\mathbf{x}) = \mathbf{b}_{n+2}(\mathbf{x}) + \mathcal{L}_{\mathbf{g}_n} \mathbf{b}_3(\mathbf{x}). \quad (47)$$

Multiple applications of the Lie operator as well as higher-order terms  $\mathbf{b}_n$  with  $n > 3$  lead to higher-order corrections and do not need to be considered here. Analogously to the energy functional, this transformation can be rewritten directly in terms of the vector field's coefficients. After a short calculation, one obtains

$$\tilde{\beta}_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)} = \beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)} + \sigma_{\mathbf{m}(2i-1)}, \quad (48a)$$

$$\tilde{\beta}_{[\mathbf{m}-\hat{\mathbf{e}}_{2i-1}](2i)} = \beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2i-1}](2i)} + \sigma_{\mathbf{m}(2i)} \quad (48b)$$

with the quantities

$$\sigma_{\mathbf{m}(2i-1)} \equiv \sum_{\substack{\mathbf{m}'' \in \mathcal{M}, \\ |\mathbf{m}''|=4, \\ \text{nonneg.}}} \left[ -(m''_{2i} - 1) \beta_{[\mathbf{m}'' - \hat{\mathbf{e}}_{2i-1}](2i)} \gamma_{[\mathbf{m} - \mathbf{m}'' + \hat{\mathbf{e}}_{2i-1}](2i-1)} \right. \\ \left. + \sum_{\substack{i'=1 \\ i' \neq i}}^d m''_{2i'} \left( \beta_{[\mathbf{m}'' - \hat{\mathbf{e}}_{2i'}](2i-1)} \gamma_{[\mathbf{m} - \mathbf{m}'' + \hat{\mathbf{e}}_{2i'-1}](2i'-1)} \right. \right. \\ \left. \left. - \beta_{[\mathbf{m}'' - \hat{\mathbf{e}}_{2i'}](2i'-1)} \gamma_{[\mathbf{m} - \mathbf{m}'' + \hat{\mathbf{e}}_{2i'-1} + \hat{\mathbf{e}}_{2i'} - \hat{\mathbf{e}}_{2i}](2i-1)} \right. \right. \\ \left. \left. - \beta_{[\mathbf{m}'' - \hat{\mathbf{e}}_{2i'-1}](2i')} \gamma_{[\mathbf{m} - \mathbf{m}'' + \hat{\mathbf{e}}_{2i'-1} + \hat{\mathbf{e}}_{2i'} - \hat{\mathbf{e}}_{2i}](2i-1)} \right) \right], \quad (49a)$$

$$\sigma_{\mathbf{m}(2i)} \equiv \sum_{\substack{\mathbf{m}'' \in \mathcal{M}, \\ |\mathbf{m}''|=4, \\ \text{nonneg.}}} \left[ (m''_{2i} - 1) \beta_{[\mathbf{m}'' - \hat{\mathbf{e}}_{2i-1}](2i)} \gamma_{[\mathbf{m} - \mathbf{m}'' + \hat{\mathbf{e}}_{2i-1}](2i-1)} \right. \\ \left. + \sum_{\substack{i'=1 \\ i' \neq i}}^d m''_{2i'} \beta_{[\mathbf{m}'' - \hat{\mathbf{e}}_{2i-1}](2i)} \gamma_{[\mathbf{m} - \mathbf{m}'' + \hat{\mathbf{e}}_{2i'-1}](2i'-1)} \right]. \quad (49b)$$

It is emphasized that  $\sigma_{\mathbf{m}(2i-1)}$  and  $\sigma_{\mathbf{m}(2i)}$  depend on the resonant coefficients  $\gamma_{\mathbf{m}k}$  linearly and that only the third-order coefficients  $\beta_{\mathbf{m}k}$  occur therein.

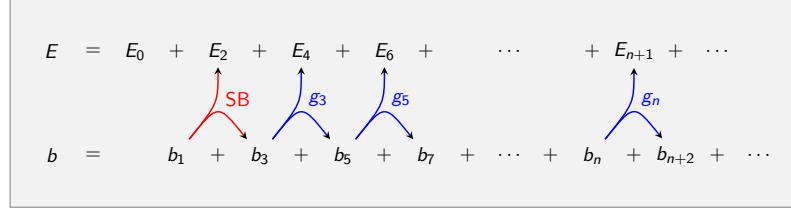
**3.3.2. Determination of the generating function's resonant coefficients** As already mentioned above, the resonant coefficients of each generating function are free parameters, in the sense that they do neither change the polynomial structure of the dynamical equations nor that of the energy functional. However, they do modify the coefficients of the respective expansions. In this section, it is shown how these resonant coefficients can be determined in a way that the dynamical equations and the energy functional fulfil the canonical equations (42), i.e. the normal form coordinates are canonical ones. This procedure works as follows (see Fig. 2):

- (i) It is assumed that Eqs. (43b) and (43c) are fulfilled for  $|\mathbf{m}| = n + 1$ , i.e. the respective term of the dynamical equations can be written as a symplectic gradient

$$\mathbf{b}_n(\mathbf{x}) = \mathcal{J} \frac{\partial}{\partial \mathbf{x}} \tilde{E}_{n+1}(\mathbf{x}) \quad (50)$$

with a scalar function  $\tilde{E}_{n+1} = \sum_{|\mathbf{m}|=n+1} \tilde{\xi}_{\mathbf{m}} \mathbf{x}^{\mathbf{m}}$ . Note that the latter does not need to be identical to the energy functional,  $\tilde{E}_{n+1} \neq E_{n+1}$ .

- (ii) Replacing  $\beta_{\mathbf{m}k} \rightarrow \tilde{\beta}_{\mathbf{m}k}$  and  $\xi_{\mathbf{m}} \rightarrow \tilde{\xi}_{\mathbf{m}}$ , Eq. (43a) with  $|\mathbf{m}| = n + 1$  as well as (43c) with  $|\mathbf{m}| = n + 2$  are used as conditional equations for the determination of the resonant coefficients of the order  $n$ . These equations form a linear system of equations with the resonant coefficients being the variables.
- (iii) By construction of step (ii), the assumption in step (i) is fulfilled in the next-higher order  $n + 2$ . Therefore, the procedure can be repeated successively for the orders  $n = 3, 5, 7, \dots$



**Figure 2.** Scheme of the procedure to determine the resonant coefficients of the generating function. In each order  $n \geq 3$ , it is assumed that the term  $\mathbf{b}_n$  of the dynamical equations fulfils Eqs. (43b) and (43c). Then, the resonant coefficients of the generating function are determined using the part  $E_{n+1}$  of the energy functional and the next-higher order term  $\mathbf{b}_{n+2}$  of the equations of motion (blue). The resonant generating function is constructed in a way that  $\mathbf{b}_n$  as well as  $E_{n+1}$  are connected via the canonical equation (42) and that Eqs. (43b) and (43c) are valid for the term  $\mathbf{b}_{n+2}$ . The whole procedure is applied successively for the orders  $n = 3, 5, 7, \dots$ . Note that the same conditions are fulfilled automatically for the terms  $\mathbf{b}_1, E_2$ , and  $\mathbf{b}_3$ , if the symplectic basis (SB; red) is made use of as discussed in Sec. 3.1.

After having calculated the term  $\tilde{E}_{n+1}$  in step (i), the system of equations in step (ii) can be set up by inserting Eqs. (46) and (48) into the Eqs. (43a) and (43c) after having replaced  $\beta_{\mathbf{m}k} \rightarrow \tilde{\beta}_{\mathbf{m}k}$  and  $\xi_{\mathbf{m}} \rightarrow \tilde{\xi}_{\mathbf{m}}$ :

$$\sum_{\substack{i=1 \\ \text{nonneg.}}}^d \lambda_i \gamma_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)} = \tilde{\xi}_{\mathbf{m}} - \xi_{\mathbf{m}}, \quad (51a)$$

$$m_{2j} \sigma_{\mathbf{m}(2i-1)} - m_{2i} \sigma_{\mathbf{m}(2j-1)} = m_{2i} \beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2j}](2j-1)} - m_{2j} \beta_{[\mathbf{m}-\hat{\mathbf{e}}_{2i}](2i-1)}. \quad (51b)$$

Equation (51a) must hold for all  $|\mathbf{m}| = n+1$  and Eq. (51b) for all  $|\mathbf{m}| = n+2$  as well as  $i, j = 1, \dots, d$  with  $i \neq j$ . Equations (51) are written in a way that all terms which depend on the resonant coefficients  $\gamma_{\mathbf{m}k}$  occur on the left-hand side, while the right-hand side is independent of these terms. Because of the fact that the resonant coefficients enter Eqs. (51) linearly according to Eqs. (49), they form a linear system of equations which can formally be written as

$$\mathcal{A}\mathcal{G} = \mathcal{B}. \quad (52)$$

Here, the matrix  $\mathcal{A}$  and the vector  $\mathcal{B}$  are both determined by the known quantities  $\beta_{\mathbf{m}k}$ ,  $\lambda_i$ ,  $\xi_{\mathbf{m}}$ ,  $\tilde{\xi}_{\mathbf{m}}$ , and  $m_k$ . All the unknown terms, i.e. the resonant coefficients  $\gamma_{\mathbf{m}k}$ , are collected in the vector  $\mathcal{G}$ . It is noted that the number of the resonant coefficients is, in general, smaller than the number of equations, so that the system (52) is overdetermined. However, it is guaranteed by Darboux's theorem that there exists a solution, because otherwise it would not be possible to construct canonical coordinates which would violate the theorem. We note that it is appropriate to solve Eq. (52) via a least-square fit  $\|\mathcal{A}\mathcal{G} - \mathcal{B}\| \stackrel{!}{=} \min$ . The minimum of this fit must be zero because of Darboux's theorem, and its actual value in a numerical implementation is a measure of success of the procedure. After the resonant coefficients of a certain degree  $n$  have been determined as the solutions of Eq. (52), the corresponding transformation needs to be applied to the full expansion, i.e. Eqs. (26) and (28) must be evaluated.



### 3.4. Canonical torus structure of the noncanonical Hamiltonian system

After the normal form expansion has been applied as discussed in Secs. 3.2 and 3.3, the normal form coordinates are canonical ones by construction. The expansions fulfil the canonical equations (42) in every order  $n$  with the energy functional acting as Hamiltonian

$$H = E(\mathbf{x}). \quad (53)$$

Because of the summation over  $\mathbf{m} \in \mathcal{M}$  in Eq. (41), this Hamiltonian only consists of monomials

$$\mathbf{x}^{\mathbf{m}}|_{\mathbf{m} \in \mathcal{M}} = \prod_{i=1}^d (x_{2i-1} x_{2i})^{m_{2i}} \equiv \prod_{i=1}^d (q_i p_i)^{m_{2i}}, \quad (54)$$

where the normal form coordinates have been interpreted pairwise as standard canonical coordinates  $q_i \equiv x_{2i-1}$  and  $p_i \equiv x_{2i}$  in the last step. Moreover, these products directly define action variables

$$J_i \equiv \begin{cases} q_i p_i, & \lambda_i = \kappa_i \quad (\kappa_i \in \mathbb{R}), \\ i q_i p_i, & \lambda_i = i \omega_i \quad (\omega_i \in \mathbb{R}), \end{cases} \quad (55)$$

where the imaginary unit in the definition compensates the respective contribution of each purely imaginary eigenvalue. With this definition, the Hamiltonian is a real function in the action variables

$$H = E(\mathbf{J}) = \sum_{n=0}^m E_n(\mathbf{J}). \quad (56)$$

If all the action variables correspond to stable oscillations of the system, and denoting the corresponding angle variables by  $\varphi_i$ , the dynamical equations are

$$\dot{\varphi}_i = \frac{\partial H(\mathbf{J})}{\partial J_i} \equiv \omega_i(\mathbf{J}), \quad (57a)$$

$$\dot{J}_i = -\frac{\partial H(\mathbf{J})}{\partial \varphi_i} = 0, \quad (57b)$$

where  $\omega_i(\mathbf{J})$  are the characteristic frequencies of the system. These have the solution

$$\varphi_i(t) = \omega_i t + \varphi_i(0), \quad (58a)$$

$$J_i(t) = \text{const.} \quad (58b)$$

This shows that, in normal form coordinates, the dynamics of the system is restricted to a  $d$ -dimensional torus  $\mathcal{T}^d$  if all eigenvalues are purely imaginary. If  $k$  of the actions (55) correspond to real eigenvalues, then the dynamics takes place on a manifold with the structure  $\mathcal{T}^{d-k} \otimes \mathbb{R}^k$ .

## 4. Variational approach to quantum systems as a noncanonical Hamiltonian system

As an exemplary field of application of the procedure to construct canonical normal form coordinates, we present in this section a variational approach to quantum

systems. The dynamics of the latter is, in general, described by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \hat{H} \psi(\mathbf{r}, t), \quad (59)$$

where  $\psi(\mathbf{r}, t)$  is the time-dependent wave function of the system and  $\hat{H}$  is the Hamilton operator. As we have already discussed above, there is a natural canonical structure inherent to this description. This becomes especially obvious, if one derives the Schrödinger equation in the framework of field theory from the Hamiltonian density

$$\mathcal{H} = \int d^3r \, \psi^\dagger(\mathbf{r}, t) \hat{H} \psi(\mathbf{r}, t) \quad (60)$$

using the functional derivatives

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \frac{\partial \mathcal{H}}{\partial \psi^\dagger(\mathbf{r}, t)}, \quad i\hbar \frac{\partial}{\partial t} \psi^\dagger(\mathbf{r}, t) = -\frac{\partial \mathcal{H}}{\partial \psi(\mathbf{r}, t)}. \quad (61)$$

This description of a quantum system is very general, however, it is often not feasible in actual applications due to the field operator's infinite number of degrees of freedom.

One possible approach to reduce the system's number of degrees of freedom is its treatment within a variational approach. Therein, the Schrödinger equation (59) is solved approximately by replacing the original wave function  $\psi(\mathbf{r}, t)$  by a trial wave function

$$\psi(\mathbf{r}, t) = \psi(\mathbf{r}, \mathbf{z}(t)). \quad (62)$$

Here,  $\mathbf{z}(t) = [z_1(t), z_2(t), \dots, z_d(t)]^\top \in \mathbb{C}^d$  is a set of complex and time-dependent variational parameters, and the time evolution of the wave function is completely determined by that of the variational parameters. In the framework of the variational approach, expectation values of the system's observables, in general, become functions depending on the variational parameters  $\mathbf{z}(t)$ . In particular, the energy functional of the system is given by the expectation value of the Hamilton operator

$$E(\mathbf{z}(t)) = \langle \psi(\mathbf{r}, \mathbf{z}(t)) | \hat{H} | \psi(\mathbf{r}, \mathbf{z}(t)) \rangle. \quad (63)$$

In order to describe the dynamics of the system in the Hilbert subspace which is spanned by the variational ansatz, we apply the Dirac-Frenkel-McLachlan variational principle [12, 13]. This claims to minimize the norm of the difference between the left- and the right-hand side of the Schrödinger equation (59),

$$I \equiv \|\dot{\psi} - \hat{H}\psi\|^2 = \langle -i\dot{\psi} - \hat{H}\psi | \dot{\psi} - \hat{H}\psi \rangle \stackrel{!}{=} \min. \quad (64)$$

Here,  $\hbar = 1$  has been set, the arguments of the wave function  $\psi$  have been omitted for brevity, and also the time dependence of the variational parameters  $\mathbf{z}$  will be dropped in the following. The quantity  $I$  is minimized with respect to  $\phi$  and  $\phi \equiv \dot{\psi}$  is set afterwards which means that the Schrödinger equation is solved within the Hilbert subspace of the variational ansatz with the least possible error. Since the approximate solution of the Schrödinger equation is intended to minimize the quantity  $I$ , the latter's variations must vanish,

$$\delta I = \langle -i\delta\phi | \dot{\psi} - \hat{H}\psi \rangle + \langle -i\dot{\psi} - \hat{H}\psi | i\delta\phi \rangle \stackrel{!}{=} 0. \quad (65)$$

Because of Eq. (62), the time derivative of the trial wave function,  $\phi = \dot{\psi}$ , and its variation  $\delta\phi$  yield

$$\phi = \sum_{m=1}^d \frac{\partial\psi}{\partial z_m} \dot{z}_m, \quad \delta\phi = \sum_{n=1}^d \frac{\partial\psi}{\partial z_n} \delta\dot{z}_n, \quad (66)$$

so that one obtains

$$\delta I = \sum_{m,n=1}^d \left\langle \frac{\partial\psi}{\partial z_m} \left| -\frac{\partial\psi}{\partial z_n} \dot{z}_n - i\hat{H}\psi \right. \right\rangle \delta\dot{z}_m^* + \left\langle -\frac{\partial\psi}{\partial z_n} \dot{z}_n + i\hat{H}\psi \left| \frac{\partial\psi}{\partial z_m} \right. \right\rangle \delta\dot{z}_m \stackrel{!}{=} 0. \quad (67)$$

We now proceed from the complex variational parameters  $\mathbf{z}$  to their real and imaginary parts  $\mathbf{x} \equiv (\mathbf{z}^r, \mathbf{z}^i)^\top \in \mathbb{R}^{2d}$ . In this case, the variations with respect to the variational parameters in Eq. (67) are not independent, and both terms together result in the dynamical equations

$$\sum_{n=1}^{2d} \text{Im} \left\langle \frac{\partial\psi}{\partial x_m} \left| \frac{\partial\psi}{\partial x_n} \right. \right\rangle \dot{x}_n = -\text{Re} \left\langle \frac{\partial\psi}{\partial x_m} \left| \hat{H}\psi \right. \right\rangle \quad (68)$$

for the time evolution of each real variational parameter  $m = 1, \dots, 2d$ . Using the property

$$\frac{\partial}{\partial \mathbf{x}} E(\mathbf{x}) = 2 \text{Re} \left\langle \frac{\partial\psi(\mathbf{x})}{\partial \mathbf{x}} \left| \hat{H} \right| \psi(\mathbf{x}) \right\rangle, \quad (69)$$

which directly follows from Eq. (63) after having replaced  $\mathbf{z} \rightarrow \mathbf{x}$  and defining the quantities

$$K_{mn} \equiv 2 \text{Im} \left\langle \frac{\partial\psi}{\partial x_m} \left| \frac{\partial\psi}{\partial x_n} \right. \right\rangle, \quad (70a)$$

$$h_m \equiv 2 \text{Re} \left\langle \frac{\partial\psi}{\partial x_m} \left| \hat{H}\psi \right. \right\rangle, \quad (70b)$$

the dynamical equations (68) immediately take the form (5). We note that the matrix  $K$  with the entries (70a) is skew-symmetric by definition, because the imaginary part changes its sign under complex conjugation of the bracket. Furthermore, the corresponding 2-form (6) is nondegenerate if  $K$  is invertible, as we have already discussed in Sec. 2. Moreover, it is closed, i.e. Eq. (7) holds, because

$$\partial_{x_k} K_{mn} = \text{Im} \left\langle \frac{\partial^2\psi}{\partial x_k \partial x_m} \left| \frac{\psi}{\partial x_n} \right. \right\rangle - \text{Im} \left\langle \frac{\partial^2\psi}{\partial x_k \partial x_n} \left| \frac{\psi}{\partial x_m} \right. \right\rangle, \quad (71)$$

with the definition (70a), and the single terms cancel out when it is summed over  $k, m, n$ .

Concluding, the variational approach to quantum systems discussed in this section defines a noncanonical Hamiltonian system for its variational parameters as we have defined it in Sec. 2. Combining the procedure presented in Sec. 3 with the variational framework, canonical normal form coordinates can be constructed in variational space in any desired order. Moreover, if transition states can be identified in a quantum system, a general transition state theory for quantum wave packet dynamics is directly

obtained by combining the variational approach and the procedure presented in Sec. 3 with the usual transition state theory in classical phase space [7]. By construction of the normal form Hamiltonian in action coordinates from the original energy functional, one can directly define a dividing surface in variational space which is free of local recrossings [14]. For applications of the procedure to the reaction dynamics of nonlocal quantum wave packets and the thermal decay of Bose-Einstein condensates, the reader is referred to Refs. [15, 16], where also the applicability of the method presented to the field on nonlinear Schrödinger equations is demonstrated. Further details on the numerical implementation of the method can be found in Ref. [17].

## 5. Conclusion and outlook

In this paper, we have demonstrated a general method to construct local, canonical coordinates in the vicinity of a fixed point of a noncanonical Hamiltonian system via normal form expansions. The method allows for the general and systematic investigation of noncanonical Hamiltonian systems in the vicinity of fixed points. Furthermore, it is applicable for systems with arbitrary degrees of freedom, in arbitrary orders of the local expansion, and it is independent of the precise form of the Hamiltonian. As a possible field of application, we have discussed a variational approach to quantum systems which defines a noncanonical Hamiltonian system for the variational parameters.

A further generalization of the method presented here can be achieved by dropping the assumption of rational independence of the eigenvalues. This step will allow to construct the system's canonical normal form also in situations with strong mode coupling of the different degrees of freedom. The general procedure presented in this paper also works in this case, however, additional terms in the normal form Hamiltonian will occur. This generalization is currently in progress. Due to the additional terms in the normal form and with the above made definition of action variables, one then expects the local canonical Hamiltonian to depend on both its action and angle variables,  $H = H(\mathbf{J}, \boldsymbol{\phi})$ , to which e.g. classical perturbation theory can be applied in a subsequent step.

## Acknowledgement

This work was supported by Deutsche Forschungsgemeinschaft. A. J. is grateful for support from the Landesgraduiertenförderung of the Land Baden-Württemberg. We thank Dario Bambusi, Marcel Griesemer, Guido Schneider, and the members of the Graduiertenkolleg 1838 "Spectral Theory and Dynamics of Quantum Systems" for fruitful discussions.

## Literature

- [1] J. S. Langer. Theory of the Condensation Point. *Ann. Phys.* **41**, 108 (1967).
- [2] J. S. Langer. Statistical Theory of the Decay of Metastable States. *Ann. Phys.* **54**, 258 (1969).
- [3] P. Pechukas. Transition state theory. *Ann. Rev. Phys. Chem.* **32**, 159 (1981).
- [4] K. J. Laidler and M. C. King. The Development of Transition-State Theory. *J. Phys. Chem.* **87**, 2657 (1983).
- [5] P. Hänggi, P. Talkner, and M. Borkovec. Reaction-rate theory: fifty years after Kramers. *Rev. Mod. Phys.* **62**, 251 (1990).
- [6] D. G. Truhlar, B. C. Garrett, and S. J. Klippenstein. Current Status of Transition-State Theory. *J. Phys. Chem.* **100**, 12771 (1996).
- [7] H. Waalkens, R. Schubert, and S. Wiggins. Wigner’s dynamical transition state theory in phase space: classical and quantum. *Nonlinearity* **21**, R1 (2008).
- [8] J. Murdock. *Normal Forms and Unfoldings for Local Dynamical Systems*. Springer, New York (2010).
- [9] F. Scheck. *Theoretische Physik 1*. Springer, Berlin (2007).
- [10] G. Darboux. Sur le problème de Pfaff. *Bull. Sci. Math.* **6**, 14–36 (1882).
- [11] V. I. Arnold. *Mathematical Methods of Classical Mechanics*. Springer, New York (1989).
- [12] J. Frenkel. *Wave mechanics. Advanced General Theory*. Clarendon Press, Oxford (1934).
- [13] A. D. McLachlan. A variational solution of the time-dependent Schrödinger equation. *Mol. Phys.* **8**, 39 (1964).
- [14] H. Waalkens and S. Wiggins. Direct construction of a dividing surface of minimal flux for multi-degree-of-freedom systems that cannot be recrossed. *J. Phys. A: Math. Gen.* **37**, L435 (2004).
- [15] A. Junginger, J. Main, G. Wunner, and M. Dorwarth. Transition state theory for wave packet dynamics. I. Thermal decay in metastable Schrödinger systems. *J. Phys. A: Math. Theor.* **45**, 155201 (2012).
- [16] A. Junginger, M. Dorwarth, J. Main, and G. Wunner. Transition state theory for wave packet dynamics. II. Thermal decay of Bose-Einstein condensates with long-range interaction. *J. Phys. A: Math. Theor.* **45**, 155202 (2012).
- [17] A. Junginger. *Transition state theory for wave packet dynamics and its application to thermal decay of metastable nonlinear Schrödinger systems*. Ph.D. thesis, University of Stuttgart (2014). Url: <http://elib.uni-stuttgart.de/opus/volltexte/2014/9478/>.